

# LC/MS/MS Library

## Strategy for Identifying Harmful Organic Compounds in Drinking Water

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### Background

The combination of liquid chromatography (LC) and mass spectrometry (MS) is a powerful tool in modern analytical chemistry. The goal of our project is to harness this current LC/MS technology to provide a library and screening method that can be used to analyze drinking water for harmful organic compounds. This library would be highly useful in emergency situations and for routine monitoring. Such a library would include classes of compounds – agrochemicals, pharmaceuticals and industrial chemicals – not readily addressed by other analytical techniques, such as GC/MS.

### Methodology

#### Building the Library

Pure chemical compounds were analyzed using a Waters® Alliance® 2695 liquid chromatograph interfaced to a Quattro micro™ mass spectrometer. From the resulting chromatograms, retention times for each compound were recorded and clean mass spectra were appended to the Library. Each Library entry includes a mass spectrum and supporting fields of information about the specific compound: CAS #, retention time, molecular formula and weight, and ionization conditions.

#### Using the Library

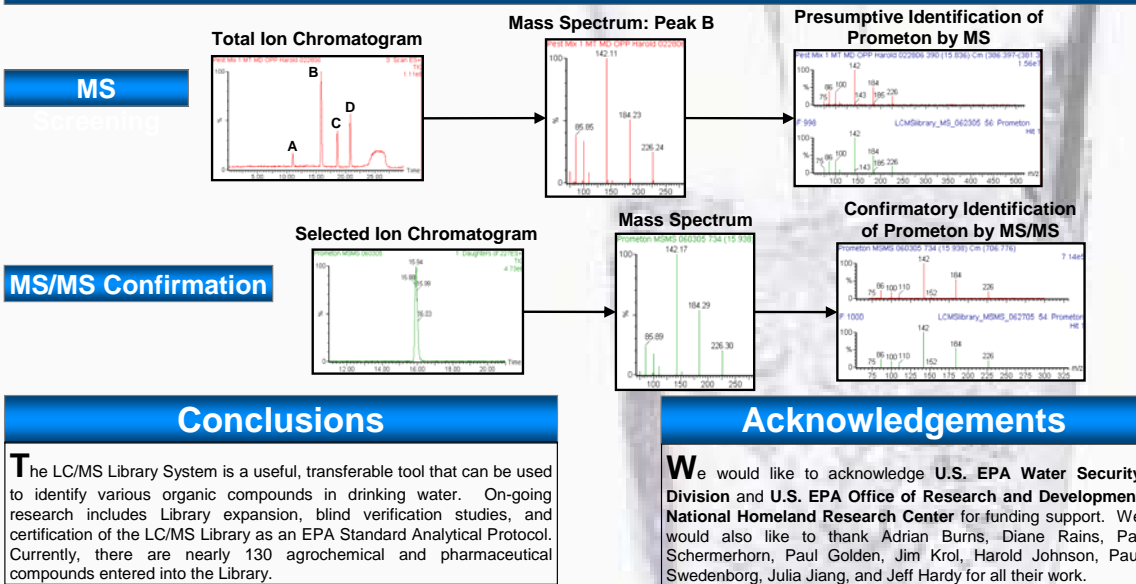
Drinking water, well water and clean surface waters can be sampled, filtered and (without a need for extraction) analyzed via LC/MS. Details of this analysis are given in the LC/MS Library System Protocol. If a peak is found, the associated mass spectrum can be referenced against the Library to identify the peak. If the LC/MS identification is ambiguous in any way, LC/MS/MS analysis can be performed to confirm or deny the identification.

### Collaborators

This project involves government and private sector cooperation. In addition to the original CRADA (cooperative research and development agreement) in place between the U.S. EPA Region 5 Chicago Regional Laboratory and Waters Corporation, other entities have become involved in collaboration. Such a list includes:

- U.S. EPA Office of Research and Development
- U.S. EPA Office of Pesticide Programs

### Data



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